

Abstract Submitted
for the DAMOP07 Meeting of
The American Physical Society

Sorting Category: 3.4 (T)

Dissociative Electron Attachment to chloroacetylene V.

NGASSAM, A.E. OREL, Department of Applied Science, University of California Davis — The production of two fragments with Σ symmetry from electron-impact dissociation of C_2H_2 , which has only a low lying π^* resonance at equilibrium geometry, has been explained by the existence of interactions with σ^* resonances at bent geometries. We are investigating the presence of such multidimensional effects in the dissociative attachment of chloroacetylene (C_2HCl). We have performed electron scattering calculations using the Complex Kohn variational method to determine the resonance energies and widths of the chloroacetylene resonances as a function of both the Cl- C_2H bond distance as well as the variation with C-C stretch and bend. We will discuss our results and our prediction of the dissociation dynamics in comparison to the findings for C_2H_2 . This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Chemical Sciences and the National Science Foundation, PHY-05-55401.

Prefer Oral Session
 Prefer Poster Session

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Date submitted: 03 Feb 2007

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